Measurements and calculations of Zn-like heavy ions: an update[1]

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Abstract: Previous observations of Zn-like ions of elements Yb ($Z = 70$) through U ($Z = 92$) in an electron beam ion trap differed (by value and by isoelectronic trend) from the (less precise) results of laser-produced plasma experiments and highlighted the need for much better calculations of ions with more than one electron in the valence shell. We review the progress since achieved and present new calculations for ions in the above range as well as EBIT observations of Zn-like Pt^{48+} ions ($Z = 78$). We identify accurate ab initio calculations that agree with the EBIT data as well as recent calculations that clearly fall short.

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Résumé : Des observations précédentes d'ions de type Zn des éléments Yb ($Z = 70$) jusquà U ($Z = 92$) dans un piège ionique à faisceau d'électrons diffèrent (en valeur et par tendance isoélectronique) de résultats (moins précis) d'expériences sur des plasmas produits par laser. Ce qui souligne le besoin pour de bien meilleurs calculs sur les ions avec plus d'un électron dans la couche de valence. Nous passons en revue les progrès faits depuis ce temps et présentons de nouveaux calculs pour des ions dans le domaine décrit au-dessus, aussi bien que les mesures sur des ions de type Zn comme Pt^{+48} ($Z = 78$) provenant de l'expérience EBIT. Nous identifions les calculs précis ab initio qui sont en accord avec les données EBIT, ainsi que des calculs récents qui sont nettement en désaccord.

[Traduit par la Rédaction]

1. Introduction

In fusion-oriented magnetically confined hot plasmas, high-Z atoms will be ionized to very high charge states, and the charge state distribution in a given location will be used as a transport diagnostic. The identification of individual spectra that contribute to the emission of a hot plasma requires both survey and specific high-resolution observations. While a growing body of data on tungsten (W, $Z = 74$), the expected dominant contaminant, is being accumulated in various laboratories or treated by collisional-radiative calculations in preparation for future observations [1–13], it seems worthwhile to also study nearby elements to ascertain the understanding of the systematics and to provide cross checks. For example, hohlraums made of gold ($Z = 79$) are being employed in inertial fusion experiments (see refs. in [14, 15]). Precision spectroscopy of $4s–4p_{3/2}$ transitions in Cu- and Zn-like ions produced and excited in an electron beam ion trap (EBIT) has encompassed Yb, W, and Au in a series of studies that reached up to U ($Z = 92$) [16–18], and very good agreement of earlier theory and later EBIT experiment was found for Cu-like ions. In contrast, relativistic calculations have been performed and adjusted to the high-density plasma observations of laser-produced plasmas [19]; these measurements and tailored calculations were later found to differ progressively from the low-density plasma trend at high Z. The semi-empirically adjusted calculations made it easy to interpolate expected results for elements not covered in the laser-produced plasma experiments, but the process also introduced the same systematic error in the calculations as has since been recognized in the experiment. Evidently, ab initio calculations are required to avoid the trappings of such self-reference. For the Cu isoelectronic sequence, an ab initio calculation with only the QED contributions adjusted semi-empirically (not to the data in question) [20] and another one with an ab initio treatment throughout [21] agreed with each other within about 100 ppm, and the latter calculations also agreed with experiment [18] up to $Z = 92$.

Meanwhile in contrast, the calculations for Zn-like ions, which used similar algorithms, nevertheless deviated pronouncedly (typically by several thousand ppm) and with different isoelectronic trends from the experimental findings.

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Even when much improved calculations of Zn-like ions [22] became available, the differences for individual elements did not follow a smooth trend. In such a situation it is not always clear whether the fault is with the experiment (for example, because of unrecognized line blends or systematic errors, as with the Cu-like ion data from laser-produced plasmas discussed above) or with theory. Au was one of the earlier experimental data points that had been studied with moderate spectral resolution only, and it was deemed wise to add data on a nearby element (Pt has $Z = 78$) as a cross check. Moreover, the previous experiments had instigated new relativistic calculations (using the MCDF approach) for Cu- through Ge-like ions from $Z = 70$ onwards, and new data might test the predictive power of these calculations.

Recently the electron beam ion trap group at NIST has also recorded data on similar ions, mostly on $4s–4p_{1/2}$ transitions. Their moderate resolution spectrograph [23] covers the range from 40 to 200 Å; some of the shorter wavelength $4s–4p_{3/2}$ transitions have been observed in second order of diffraction. At the Livermore EBIT, a more highly resolving spectrograph is available. We describe our measurement of EUV emission by highly charged Pt ions, report on a new calculation of the level structure of Pt^{48+} ions and some similar ions of nearby elements using a relativistic multireference Møller–Plesset code, and review the state of the art of measurements and calculations for Zn-like ions from Yb^{40+} to U^{62+}.

2. Experiment

The experiment was performed at the EBIT-I [24] at the Lawrence Livermore National Laboratory. The device has been optimized for spectroscopic studies of highly charged ions [25]. Pt was introduced to ultra-high vacuum of the EBIT in the form of a wire probe [26, 27], the tip of which was eroded by ion sputtering. Every 20 to 60 s, the content of the trap was dumped to halt the accumulation of possible contaminants, such as barium and tungsten, and then the trap cycle was repeated. The measurements were run parasitically alongside another experiment that involved many different electron beam energy settings, most of them below optimum for the production of Zn-like ions. Only those data sets that had an electron beam energy in the range 2 to 5 keV were considered for the present analysis; in these data sets, Ni-like ions (Pt^{50+}, IP = 4724 eV) and Cu-like ions (Pt^{49+}, IP = 2848 eV) represented the highest charge states, while Ga- and Ge-like ions (Pt^{48+}, Pt^{47+}) were present in at least the same but in most cases higher abundance. The Livermore EBIT group uses a microcalorimeter spectrometer [28] that monitored the ion charge state distribution in the trap by ways of the X-ray emission.

Prominent $4s–4p_{3/2}$ transitions in Cu- through As-like ions are expected at wavelengths near 50 Å. In this wavelength range, calibration lines of B, N, and Ar are available, although not conveniently close. A previously described grazing-incidence flat-field spectrograph [29] was used that has since undergone modifications to extend its wavelength coverage. This range extension was used to try to see the Pt lines of interest in second-diffraction order, using oxygen (O VI [30]) and neon (Ne VI–VIII [31–35]) lines for calibration. The spectrograph has an $R = 44.3$ m variable spacing grating and is equipped with a cryogenic CCD detector.

Fig. 1. Section of an EUV spectrum of Pt recorded at the Livermore EBIT. The data for this spectrum have been co-added from several spectra recorded at different electron beam energy settings. The lines marked Pt and (II) are second diffraction order images of Pt in various charge states identified by the respective isoelectronic sequence. Further line assignments are in progress.

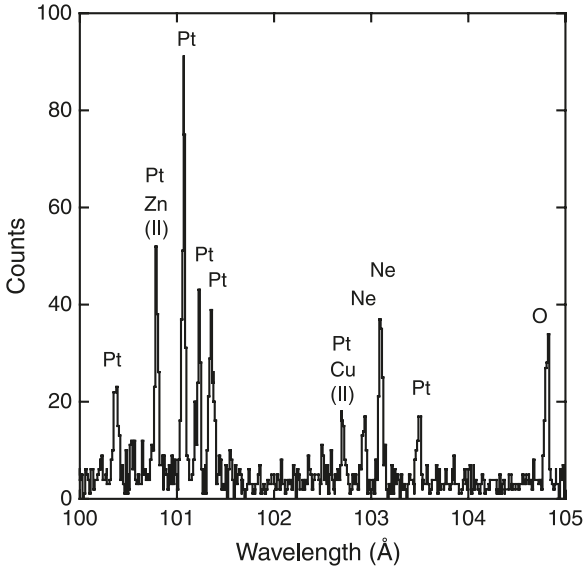


Figure 1 shows a section of an EUV spectrum summed from several 60 min exposures of a cryogenic CCD camera and at different electron beam energy settings. The line width (FWHM) is 50 mÅ, corresponding to a resolving power of 2000. Because of the given charge state balance, the resonance line of the Cu-like ion appears rather weakly, but the counting statistics are good enough to determine the (first-order) wavelength to 51.350 ± 0.003 Å. This is in excellent agreement with the isoelectronic trend of the previous Livermore EBIT data [18] relative to the predictions by Kim et al. [20]. The line at 50.390 ± 0.003 Å is identified with the resonance line in the Zn-like ion of Pt. Additional lines (Table 1) from transitions, presumably in Ga- and Ge-like ions, are in the process of being identified on the basis of isoelectronic systematics and of various calculations. The results will eventually be presented elsewhere.

3. Calculation

Since the latest experimental report on Zn-like ions of heavy elements [36], a number of new calculations has been published. Vilkas and Ishikawa [22] have applied the multireference Møller–Plesset (MR-MP) formalism, Blundell et al. [37, 38] and very recently Safronova and Safronova [39] have used many-body perturbation theory, Quinet et al. [40] have produced results from multiconfiguration Dirac–Fock calculations, and Cheng and Chen have employed relativistic configuration interaction calculations [41]. We again rely on the MR-MP code that was developed in the group of Y. Ishikawa to treat the structure of many-electron ions with high accuracy [42–45]. When this code was previously used by Vilkas and Ishikawa [22] on Zn-like ions, it employed an "optimized" (limited) basis set to accommodate limited computing resources. With such a relatively small basis set, the results may to some degree depend on the basis set chosen.

Table 1. Energies of the 14 lowest levels of Zn-like ions as calculated by multireference Møller–Plesset code (see text).

				Energy (cm^{-1})				
Index	Config.	Parity	J	Yb^{40+}	W^{44+}	Os^{46+}	Pt^{48+}	Au^{49+}
1	$4s^2$	even	0	0	0	0	0	0
2	4s4p	odd	0	627 674	697 859	734 126	771 173	790 002
3	4s4p	odd	1	676 609	753 227	792 719	833 000	853 451
4	$4p^2$	even	0	1 227 801	1 504 724	1 663 845	1 755 554	1 797 675
5	4s4p	odd	2	1 354 778	1 591 325	1 672 614	1 838 490	1 932 092
6	4s4p	odd	1	1 433 672	1 641 209	1 805 143	1 984 643	2 080 688
7	$4p^2$	even	1	1 988 548	2 348 094	2 549 783	2 767 834	2 883 469
8	$4p^2$	even	2	1 999 517	2 360 168	2 562 396	2 780 977	2 896 873
9	4s4d	even	1	2 393 365	2 782 605	2 998 348	3 229 938	3 352 146
10	4s4d	even	2	2 413 864	2 809 859	3 028 597	3 263 093	3 386 735
11	4s4d	even	3	2 519 613	2 952 949	3 194 651	3 455 080	3 592 853
12	4s4d	even	2	2 529 622	2 998 051	3 250 012	3 517 918	3 658 752
13	$4p^2$	even	2	2 675 681	3 210 172	3 526 507	3 876 837	4 065 289
14	$4p^2$	even	0	2 677 815	3 250 287	3 577 906	3 936 626	4 128 569

There also is a much bigger basis set, the so-called universal Gaussian basis set [46] — a single, nearly complete set of basis functions applicable to many atomic systems all the way up to Lr or Rf. If one uses a smaller set of Gaussian basis functions, a tedious process of fine-tuning the basis exponents is required. This (human) labor-intensive process is no longer needed if one uses that single set of universal Gaussian basis functions, and the results seem very accurate. Our latest calculations, following the MCDF/CI/MR-MP process, used the even-tempered set 34s32p30d28f26g… With this nearly complete set of basis spinors, the calculated wavelength of the $4s^2\ {}^1S_0$–$4s4p\,{}^1P_1{}^o$ transition in Zn-like gold is 48.0610 Å, agreeing within experimental error with the experimental value of 48.0583(49) Å [14]. The earlier MR-MP calculation [22] using a smaller, less complete basis set (26s24p20d18f15g…), gave the wavelength 48.0653 Å, with a greater deviation from experiment. Similar full-scale calculations of the $4s^2\ {}^1S_0$–$4s4p\,{}^1P_1{}^o$ transition in Zn-like Pt were undertaken before the new experimental result was revealed, and the MR-MP calculated wavelength of 50.3869 Å again agrees well with experiment. Since the Au result had improved from the earlier work, energy level values were recalculated for Zn-like ions of more elements. Table 1 lists the results for the first 14 levels (up to $4p^2$ and 4s4d) for five elements from Yb through Au ($Z = 70$–79). The resonance line wavelengths from this type of calculation are included in the tabulation for elements Yb through U ($Z = 70$–92, Table 2), which is discussed in the next section.

4. Comparison of measured data with calculational results

The results of measurements and calculations for the 4s2–$4s4p_{3/2}$ resonance line in Zn-like ions of Yb through U are listed in Table 2. Not all of the early calculations have been listed here (for more of the earlier refs., see [18, 36]). For the benefit of this discussion, a selection of the calculational results has been plotted, with preference to calculations that treat many elements in the isoelectronic sequence. Figure 2 shows a selection of earlier calculations (published in 2008 or before), compared with the results of our present ones. Evidently, the (ab initio) MCDF calculations by Quinet et al. [40] are better than the earlier HULLAC calculations [52] by Brown et al. [47], although they still do not agree well with experimental findings. Much closer to experiment, however, especially at the highest Z values, are the earlier MCDF results obtained by Cheng and Johnson [48]. In contrast, the more recent results obtained by Blundell [37] deviate more from experiment at the highest Z than they do, for example, at $Z = 70$. The earlier MR-MP calculations by Vilkas and Ishikawa [22] on average are closest to experiment, but they display an oscillatory behaviour compared with the trends of other computations (which probably reflects the basis set size effect mentioned in the preceding section). For $Z = 74$ and 76, the results seem too small, and beyond $Z = 79$ they appear to be slightly, but systematically, too large.

Figure 3 compares the 2009 and 2010 calculations [38, 39, 41] with our own work. Because of the much better agreement with each other, these calculations and the measurements are displayed on an expanded scale. On this scale we note slight oscillations of the difference of the results by Safronova and Safronova [39] and by Chen and Cheng [41] from ours, which probably reflects a persisting nonlinear trend in our results. In fact, the highly accurate measurements on Th and U agree even better with the RCI calculations by Chen and Cheng than with our own. On average, the mutual agreement of the updated MBPT [38], RCI [41], and our latest MR-MP calculations, as well as the agreement with experiment, are within 100 ppm. However, the data points for Os ($Z = 76$) [36] and Pb ($Z = 82$) [17] disagree with those calculations by about three standard deviations. This suggests the presence of underestimated problems and error in the experiment (of the order of a small fraction of a line width), and additional experimental data are warranted.

The most recent Safronova and Safronova MBPT results [39] are almost identical to those presented by Blundell et al. a few years earlier [37], but without the significant improvements made by Blundell since [38]. However, the new calculations have the advantage of a less restricted selection

Table 2. Predicted and measured wavelengths of the $4s^2\ ^1S_0$–$4s4p^1\ P_1^o$ transition in Zn-like ions.

Element	Z	Theory	Experiment	Element	Z	Theory	Experiment
Yb	70	73.430[a]	73.792(20)[b]	Pb	82	41.7[c]	41.689(20)[b]
		73.8[c]	73.8070(66)[d]			41.483[e]	41.7185(45)[d]
		73.368[e]				41.708[f]	
		73.784[f]				41.681[g]	
		73.823[h]				41.952[i]	
		73.790[j]				41.719[h]	
		73.464[k]				41.702[j]	
		73.816[l]				41.584[k]	
		73.8128[m]				41.729[l]	
		73.8045[n]				41.7308[m]	
		73.790[o]				41.7287[n]	
						41.701[o]	
W	74	60.629[a]	60.900(20)[b]				
		61.0[c]	60.9300(54)[d]	Bi	83	39.8[c]	39.792(20)[b]
		60.585[e]				39.578[e]	39.8151(20)[p]
		60.907[f]				39.796[f]	
		60.806[g]				39.804[h]	
		61.076[i]				39.789[j]	
		60.962[h]				39.680[k]	
		60.906[j]				39.816[l]	
		60.676[k]				39.8176[m]	
		60.935[l]				39.8150[n]	
		60.9307[m]				39.789[o]	
		60.9289[n]					
		60.906[o]		Th	90	28.6[c]	28.702(20)[b]
						28.52[e]	28.7227(67)[b]
Os	76	55.4[c]	55.3840(50)[p]			28.704[f]	28.7303(11)[p]
		55.084[e]				28.707[g]	
		55.373[f]				28.723[h]	
		55.421[h]				28.702[j]	
		55.371[j]				28.639[k]	
		55.178[k]				28.729[l]	
		55.400[l]				28.7275[m]	
		55.3973[m]				28.7293[n]	
		55.3971[n]				28.702[o]	
		55.371[o]					
				U	92	26.1[c]	26.157(20)[b]
Pt	78	50.4[c]	50.390(3)[q]			25.975[e]	26.1868(36)[d]
		50.103[e]				26.152[f]	26.1861(10)[p]
		50.365[f]				26.168[g]	
		50.584[i]				26.401[i]	
		50.196[k]				26.184[h]	
		50.3869[m]				26.160[j]	
		50.3857[n]				26.106[k]	
		50.360[o]				26.186[l]	
						26.1843[m]	
Au	79	48.0[c]	48.063(20)[b]			26.1874[n]	
		47.787[e]	48.0583(49)[d]			26.159[o]	
		48.038[f]					
		47.991[g]					
		48.266[i]					
		48.065[h]					
		48.034[j]					
		47.883[k]					

Table 2 (*concluded*).

Element	Z	Theory	Experiment	Element	Z	Theory	Experiment
		48.062[l]					
		48.0610[m]					
		48.0596[n]					
		48.033[o]					

Note: All wavelength values are in Å.

[a]Multi-configuration Dirac–Fock (MCDF) [49]
[b]Laser-produced plasma [47]
[c]Semi-empirical analysis of experimental data [50]
[d]Electron beam ion trap [17]
[e]HULLAC [47]
[f]HULLAC with semi-empirical correction [47]
[g]MCDF with QED, including nuclear size effects [48]
[h]Multireference Møller–Plesset [22]
[i]Multi-configuration random phase approximation (MCRRPA) [51]
[j]Many-body perturbation theory (MBPT) [37]
[k]MCDF [40]
[l]MBPT [38]
[m]Multireference Møller–Plesset (This work)
[n]Relativistic configuration interaction (RCI) [41]
[o]Relativistic MBPT [39]
[p]Electron beam ion trap [18]
[q]Electron beam ion trap (This work)

Fig. 2. Comparison of pre-2009 results from various computations with the results of our own MR-MP calculations (represented by the base line at zero). The range of the experimental data (see Fig. 3) lies in the bottom section of this diagram, with the Livermore EBIT data close to the base line. From the top: HULLAC calculations by Brown et al. [47]; MCDF calculation by Quinet et al. [40]; MCDF calculation by Cheng and Wagner [48]; MBPT calculation by Blundell et al. [37]; MR-MP calculation by Vilkas and Ishikawa [22].

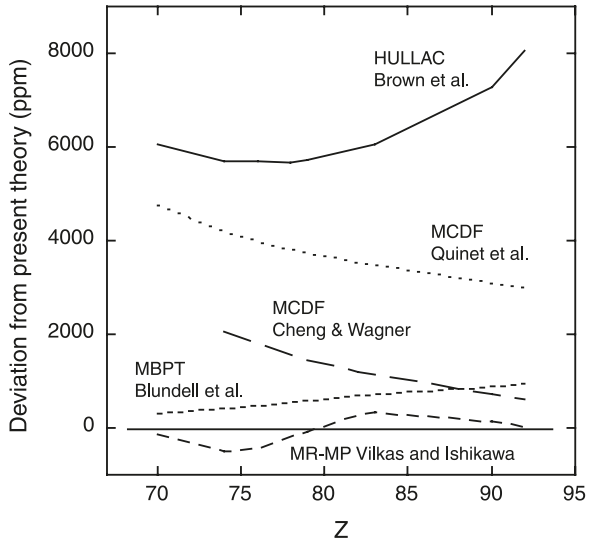
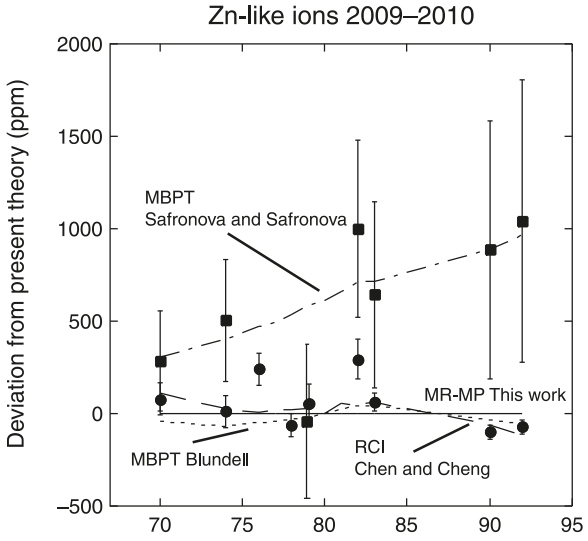


Fig. 3. Comparison of recently calculated results (published in 2009 and 2010) from various computations and measurements with the results of our own MR-MP calculations (horizontal reference line at zero). Theory: MBPT calculations by Blundell [38] and by Safronova and Safronova [39]; RCI calculation by Chen and Cheng [41]; laser-produced plasma measurements [47] (■); EBIT measurements [17, 18, 36] (●); and this work. Evidently, the laser-produced plasma measurements (except for one low data point) fall onto an isoelectronic trend curve different from that of the EBIT data. Two of the EBIT data points (for $Z = 76$ and 82) lie higher than the rest; the new data point for $Z = 78$ corroborates the trend close to the reference calculations.



of elements covered. Both of these MBPT calculations happen to agree very well with the trend of the laser-produced plasma data [47], which, however, appear to suffer from a systematic error as well as carrying considerably larger uncertainties than the (low-density, stationary ion cloud) EBIT data. Hence for practical purposes these new MBPT calculations do not represent any improvement over the older calculations presented by Brown et al. [47] and their empirical adjustment. There is a useful byproduct of the new calculations in that the intercomparison of the latest calculations shows very smooth trends and thus the likely absence of computational or clerical error in the listing of the results for any individual element.

5. Discussion

The agreement of the results of Chen and Cheng's RCI calculations [41] and of the MBPT calculations with improved QED treatment by Blundell [38] with our MR-MP calculations and the EBIT measurements of the singlet resonance line in Zn-like ions is now practically as good as for the best calculations and data in the Cu isoelectronic sequence. This is a major improvement over the situation of only two years ago. These three calculations are now accurate enough to point out which experimental data should be re-investigated ($Z = 76$ and 82). Production date, however, is no guarantee of accuracy of calculation: several fairly recent calculations of Zn-like ions are clearly poorer than some earlier ones. While MCDF calculations (such as those by Quinet et al. [40]) were known to be possibly less accurate than wanted for Zn-like ions, MBPT calculations have been among the most accurate ones for various ion species. Here we find that the fairly recent MBPT calculations by Blundell et al. [37] and by Safronova and Safronova et al. [39] practically coincide with the trend of the laser-produced plasma results, i.e., they agree with data that have been found to be systematically flawed, and disagree, in particular at the highest nuclear charges, with accurate experimental data from electron beam ion traps. We note that from the same earlier collaboration at Notre Dame [37] one later paper reports significant improvements [38], while another (even later) one more or less replicates the earlier calculations [39].

Even better measurements to reduce the scatter as well as data on more elements are required to improve the collection of reference data. The latest calculations indicate which earlier measurements might benefit most from a fresh attempt. An obvious problem with several of the existing calculations (beyond their rather limited accuracy) is that they do not cover all elements; having been published only after experimental data became available, some calculations miss the chance of displaying predictive power.

While for the Zn-like ions a new high level of accuracy has been demonstrated that matches that of calculations of Cu-like ions, the situation is clearly worse for atomic systems with more than two electrons in the valence shell. In the spectrum of Pt (Fig. 1), there are a number of other lines that are assumed to arise from Pt ions with three or four, and possibly even five or more, electrons in the valence shell. None of the published calculations can match these lines within 0.2 Å (4000 ppm). Our own exploratory MR-MP calculations suggest a number of identifications within less than 1000 ppm, which is much better than what has been available in the literature but is not yet approaching the 100 ppm accuracy now demonstrated for the Zn isoelectronic sequence. These results will be presented elsewhere [53].

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